

# Modeling and simulation of helium behavior in tungsten: A first-principles investigation



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## ABSTRACT

Tungsten (W) is regarded as the most promising candidates for plasma-facing materials (PFMs) in future fusion reactors. However, W will be exposed to high fluxes of helium (He) plasma in a nuclear fusion environment, which will degrade the thermal and mechanical properties of W. We have investigated the behavior of He in W using a first-principles method based on density functional theory. It has demonstrated that the quantitative stress indicator and the qualitative hard-sphere model can be used to characterize the effective volume and the stability of interstitial He in W. The hydrostatic tensile (compressive) strain will enhance (suppress) the dissolution and diffusion of He in W. The existing of He will have negative effect on the ideal strength of W. Vacancies and grain boundaries defects in W can serve as trapping centers for He, because the defects can provide large space for He. He will spontaneously form He clusters at the near surface by self-trapping. The pre-existing impurity/alloying element can significantly reduce the solution energy of He in W due to the electron density redistribution induced by them, such as C and Nb. The results will provide good reference for developing W materials as PFMs. This paper reviews our recent findings regarding the behavior of He in W.

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## 1. Introduction

Energy shortage is one of the most serious problems facing mankind today, which has driven us to spend great efforts to develop new energy. Nuclear fusion energy, as an environmentally friendly and abundant energy source, has been considered as one of the most important solutions to energy crisis. Nowadays, fusion energy is being developed universally via the International Thermonuclear Experimental Reactor (ITER) Project [1], which aims to demonstrate the extended burn of deuterium–tritium (D–T) plasma in a fusion reaction. The successful development of fusion energy is mainly dependent on the research of suitable component materials in the thermonuclear fusion device “Tokamak”, in which the choice of the plasma-facing materials (PFMs) is one of the key issues. PFMs will be irradiated by high energy neutrons, helium (He) and hydrogen (H) isotope plasma in fusion environment, leading to displacement damage, blistering, erosion, etc.

Tungsten (W) and W alloys are regarded as the most promising candidates for PFMs in ITER, DEMO and other future fusion reactors, owing to their high melting temperature, good thermal conductivities, and low sputtering erosion [1–4]. However, as a PFM, W will be exposed to high fluxes of He plasma in a nuclear fusion

environment, leading to retention of He, He bubbles, and fuzz nanostructure in W at different surface temperature [5–10]. Notably, this will change the properties of PFMs [11,12], such as reducing mechanical stability and thermal conductivity, thus reducing the lifetime of the W-based PFM. Therefore, as the key concerns for W-PFM, the mechanical and thermal properties under He irradiation have been under intensive investigation.

Now, it is feasible to employ the modeling and simulation method to investigate the behavior of He in W and its effect on the properties of W due to the rapid development of advanced algorithms and computing capability. Modeling and simulation plays an increasingly important role in investigating the behavior of impurity in materials. Recently, our group has investigated the behavior of He in W using first-principles method based on density functional theory, including the behavior of He in W without and with defects, and the interaction between He and other impurities in W. Here, we review them in this paper.

## 2. He behavior in intrinsic W

### 2.1. He stability

A single He atom can occupy three possible sites in metals, including the substitutional site, the tetrahedral interstitial site (TIS), and the octahedral interstitial site (OIS). Here, only

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interstitial case is considered for He, because the radius of He is much smaller than that of W. He, as a typical closed shell electronic structure element, has very weak chemical bonding with host W atoms. Therefore, the stability of He in W should be well characterized by its “effective volume”, which is determined by its atomic size relative to the available volume provided by the given interstitial site. Conventionally, the effective volume of He at the OIS is considered to be larger than that at the TIS in W (Fig. 1). This indicates that He should prefer to occupy the OIS instead of the TIS. However, it is found that the solution energy of He at the TIS is lower than that at the OIS based on first-principled calculations [13–16], which suggests He is energetically favorable sitting at the TIS rather than the OIS in W. This phenomenon also occurs in other bcc metals [14–16]. The unexpected occupation of He in bcc metals leads to a series of investigations. For example, Zu et al. attributed the TIS preference of He to the strong hybridization between the He *p* states and transition metal *d* states [15], but it is questioned by Fu and Willaime [16], due to the closed shell structure of He.

Interestingly, it is found that the qualitative judgement of the He effective volume in metals is very dependent on the empirical lattice models. Three different empirical lattice models have been taken into account to estimate the available volume of He in W [17], including the point-lattice model, the Voronoi polygon, and the hard-sphere model. According to the point-lattice model, the TIS volume is smaller than OIS volume (Table 1), contradicting with the first-principles results of He solution energies and occupation. The Voronoi model shows that the TIS volume is only slightly larger than the OIS volume. Further, the hard-sphere model predicts that the TIS volume is much larger than the OIS volume, in agreement with the first-principles results. Therefore, the hard-sphere model is a better choice to estimate the effective volume of He in metals without doing any calculation.

Most importantly, we propose a stress indicator of effective volume and stability of He in metals [17]. Here, the stress indicator is the lattice stress induced by the embedded He atom, because of the mismatch between the size of He atom and the available volume provided by the interstitial site. An equilibrium lattice is stress free. When a He atom is introduced at an interstitial site, the equilibrium state will be destroyed. Then, He will induce a lattice stress, which depends on both the atomic size effect and the electronic effect. Furthermore, the solution energies of He can be derived

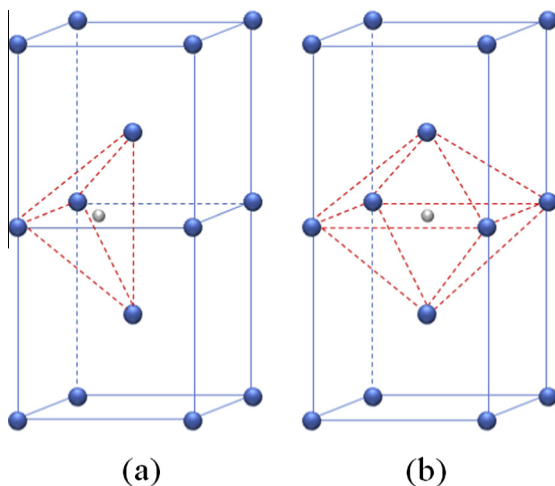


Fig. 1. The interstitial sites in body-centered cubic W, (a) the TIS and (b) the OIS. The larger blue spheres represent the W atoms, while the smaller gray spheres represent the He atoms. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1

Interstitial volume in units of  $a_0^3$  based on different lattice models, where  $a_0$  is the lattice constant [17].

Lattice model	$V_{\text{TIS}}$	$V_{\text{OIS}}$	$V_{\text{TIS}}/V_{\text{OIS}}$
Point-lattice	1/12	1/3	0.25
Voronoi	0.2568	0.2511	1.02
Hard-sphere	0.0084	0.0013	6.46

from the calculated stress tensor according to the elastic theory [18]. Relatively, the elastic stress model predicts that He prefers to occupy the TIS rather than the OIS in W, which is in good agreement with the DFT results, although there is difference of the absolute value between the individual solution energy derived from the stress model and the DFT results. The stress model also successfully predicts the occupation behavior of He in other bcc metals, as listed in Table 2. This demonstrates that the stress model prediction correlates closely with the solution energy. We believe that the quantitative lattice stress model can be used not only to interstitial cases, but also to other defects.

## 2.2. Effects of strain on He dissolution and diffusion

The initial gas pressure in He bubbles can reach several GPa [19,20], which will lead to deformation to the lattice surrounding the bubbles. Further, the subsequent He entering the bubbles must pass through the deformation (strain) region. Therefore, the effects of strain on He dissolution and diffusion is regarded as an important factor affecting He bubble formation and growth.

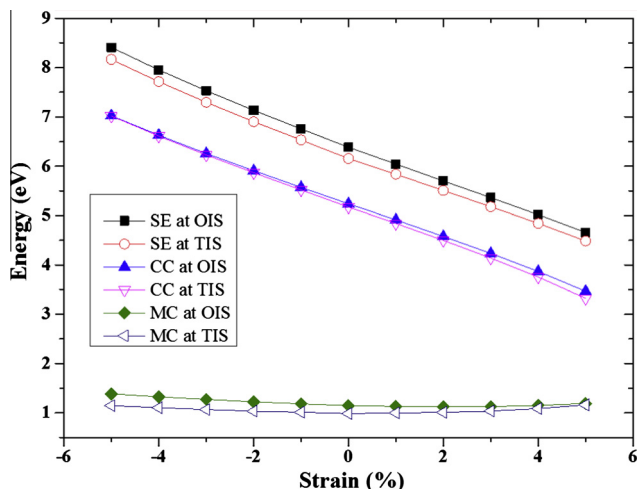
We have investigated the effects of hydrostatic strain on He dissolution and diffusion using a first-principles method [21]. It is found that the He solution energy at the TIS and the OIS monotonically decreases with the increasing tensile strain, while increases with the increasing compressive strain, as shown in Fig. 2. This suggests that the tensile will facilitate the dissolution of He in W, but the compressive strain will suppress that. Further, the He solution energy at the TIS is always lower than that at the OIS, suggesting that the TIS remains to be the energetically preferable site for He under the hydrostatic strain.

In order to explore the physical origin of He stability under the hydrostatic strain, we decompose the solution energies into two contributions. One is the deformation energy induced by the embedded He atom, defined as the energy release during the course of metal relaxation after He is removed, and called the *mechanical contribution* (MC). The other is the electronic effect, called the *chemical contribution* (CC). Fig. 2 shows the variation of the CC is similar to that of solution energy under the hydrostatic strain, while the variation of the MC is slight. The relative stability of He is dependent on the difference of solution energy between He at the TIS and the OIS, which also consists of the MC and the CC. It

Table 2

Solution energy (in eV) of He, the He-induced stress (in GPa), and solution energy of He given by elastic calculations at the TIS over OIS in bcc metals [17].

		W	Mo	Fe	Cr	V	
Solution energy	TIS	6.13	5.21	4.56	5.18	3.05	
	OIS	6.37	5.41	4.77	5.38	3.28	
$\sigma$	TIS	XX	-1.97	-1.79	-2.54	-2.29	-1.31
		YY	-1.87	-1.76	-2.61	-2.59	-1.79
		ZZ	-1.97	-1.79	-2.54	-2.29	-1.31
	OIS	XX	-1.58	-1.48	-2.38	-1.98	-1.59
		YY	-1.58	-1.48	-2.38	-1.98	-1.59
		ZZ	-2.89	-2.55	-3.24	-3.44	-1.81
Solution energy (derived)	TIS	0.10	0.09	0.22	0.16	0.11	
	OIS	0.12	0.11	0.25	0.18	0.14	



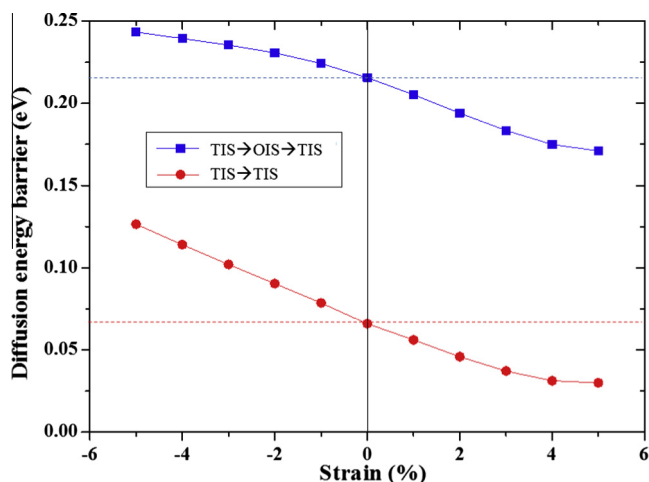
**Fig. 2.** The solution energy (SE) of He, the *mechanical contribution* (MC), and the *chemical contribution* (CC) between He at the TIS and the OIS in W as a function of strain. The MC corresponds to the deformation energy induced by the embedded He atom, and the CC represents the electronic effect for He dissolution in W [21].

is found that the MC plays a key role in the He stability in the range of  $-5\%$  to  $3\%$ , while the CC determines that in the range of  $3\%$ – $5\%$ .

Further, we investigate the effect of strain on the diffusion energy barrier of He in W. It is found that the diffusion barrier monotonically decrease (increase) with increasing tensile (compressive) strain for the TIS  $\rightarrow$  OIS  $\rightarrow$  TIS path and the TIS  $\rightarrow$  TIS path, as shown in Fig. 3. This can be attributed to that the He–W interaction will change to be weaker (stronger) with the increasing tensile (compressive) strain, thus making the diffusion of He in W easier (harder). The diffusion barrier of the TIS  $\rightarrow$  TIS path is always lower than that of the TIS  $\rightarrow$  OIS  $\rightarrow$  TIS path under all strain, which suggests the TIS  $\rightarrow$  TIS path remains to be the preferred diffusion path of He.

### 2.3. He effects on the ideal strength

Although the solubility of He in metals is extremely low, it can lead to significant changes in mechanical properties of metals [22,23]. The ideal tensile strength is the maximum tensile stress



**Fig. 3.** He diffusion energy barriers via the TIS  $\rightarrow$  TIS path and the TIS  $\rightarrow$  OIS  $\rightarrow$  TIS path as a function of applied hydrostatic strain, respectively. The TIS  $\rightarrow$  TIS path connects two TIS's directly, while the TIS  $\rightarrow$  OIS  $\rightarrow$  TIS path starts from a TIS, passes through an OIS and ends at another TIS [21].

required to yield or break a perfect crystal, which can be predicted by the first-principle computational tensile test (FPCTT). In order to evaluate the effect of He on the mechanical properties of W, the ideal strength of W with and without He have been investigated [24]. In the FPCTT, a tensile (uniaxial) strain has been applied to the chosen crystalline direction, and the corresponding stress is calculated according to the Nielsen–Martin scheme [25,26]. The tensile stress  $\sigma$  is calculated from

$$\sigma = \frac{1}{\Omega(\varepsilon)} \frac{\partial E}{\partial \varepsilon} \quad (1)$$

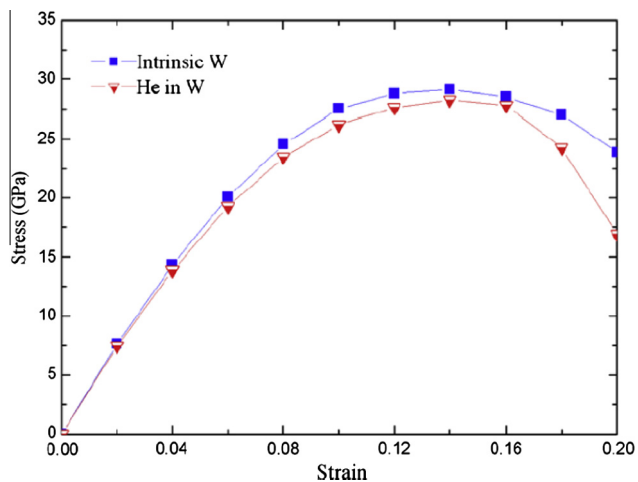
where  $E$  is the total energy and  $\Omega(\varepsilon)$  is the volume at a given tensile strain. The Poisson ratio has been considered during calculation.

Fig. 4 shows the stress–strain curve of W without and with He atom. For the intrinsic W, it can be found that the tensile stress until a strain of  $14\%$ , at which the stress reaches a maximum  $29.1$  GPa. After  $14\%$ , the stress decreases gradually. Hence, the perfect W crystal can be considered as broken after  $14\%$ , and the maximum tensile stress of  $29.1$  GPa is the ideal tensile strength. This is consistent with the previous studies [27,28]. When an impurity He atom is doped in W, the ideal tensile strength decreases to  $28.2$  GPa, which is about  $3.1\%$  lower than that of intrinsic W, as shown in Fig. 4. This suggests that the existing of He atom will degrade the mechanical properties of W. We further investigate the atomic configuration in order to explore the physical origin the degradation induced by He. It is found that the degradation can be attributed to the formation of a local bond-breaking region around the He atom during the tensile process. Further, it can be predicted that He cluster will have significant effect on the mechanical properties of W, which is easily formed due to the self-trapping of He [13].

## 3. He behavior at defects in W

### 3.1. He at vacancies

Helium prefers to occupy the defects with large space in comparison with the interstitial sites in metals, due to the closed shell structure of He. Vacancy, the typical point defect in metals, plays a key role in the dissolution and nucleation of He in W [29,30]. We have investigated the dissolution and diffusion of He in vacancy using a first-principles method [31]. It is found that vacancy centre



**Fig. 4.** The stress as a function of tensile strain by the first-principle computational tensile test for the intrinsic W and the W with He atom. The maximum tensile stress of the intrinsic W and the W–He is  $29.1$  GPa and  $28.2$  GPa at the same strain of  $14\%$ , respectively [24].

is the most stable site of He in vacancy, because there is the lowest electron density ( $\sim 0.03 \text{ e}\text{\AA}^{-3}$ ). The solution energy of He in vacancy is 1.57 eV, which is 4.59 eV lower than that of He at the TIS. This suggests that He energetically prefers to segregate towards the vacancy. Therefore, vacancy can serve as a trapping centre for He.

Kinetically, we investigated the diffusion process of He jumping in vacancy from interstitial site. As shown in Fig. 5, the TIS  $\rightarrow$  TIS path is the optical diffusion path of with a diffusion barrier of 0.06 eV for He away from the vacancy. It is found that the He diffusion barrier is reduced to 0.04 eV via the path TIS (3NN, site 1)  $\rightarrow$  TIS (2NN, site 2), and it is further reduced to 0.02 eV via the path TIS (2NN, site 2)  $\rightarrow$  TIS (1NN, site 3). This suggests that the diffusion of He will become easier and easier, when He moves closer to a vacancy. Interestingly, there is no diffusion barrier via the path TIS (1NN, site 3)  $\rightarrow$  vacancy, and thus He will experiences a downhill 'drift' diffusion into vacancy. These suggest He can very easily diffuse into the vacancy.

### 3.2. He at grain boundaries

As the regions of transition between two adjacent crystal lattices, the grain boundaries (GBs) have different chemical composition and crystallographic structure in comparison with the bulk. Thus, the properties of GB powerfully affect the chemical and physical behaviors of the whole materials [32]. The GBs is also one of the main nucleation regions of He in W. The dissolution and segregation behaviors of a single He atom at all possible interstitial and substitutional sites at GB have been investigated [33]. At pure W  $\Sigma 5$  (3 1 0)/[00 1] GB, it is found that a single He energetically prefers to occupy the substitutional site with a solution energy of 3.06 eV, which is much lower than that of He in bulk W. The segregation energy of He in W GB is calculated to be  $-1.37$  eV, which suggests that He is energetically favorable to segregate in W GB. In addition, the lowest solution energy in all the interstitial sites at GB is 3.30 eV, which is also lower than that of He in bulk. Therefore, the segregated He can occupy the substitutional or interstitial site at GB.

We further investigate the atomic configuration of GB, in order to explore the origin for He segregation at GB. As mentioned above, He exhibits a closed-shell electric structure, and thus it is favorable to sitting at the sites with larger space. Both substitutional and interstitial sites at GB can provide larger space than those in the bulk, and thus He prefers to stay in GB. Moreover, the segregated

He will induce the expansion of GB. The variation of structure induced by He will have significant effect on the mechanical properties of the W GB.

### 3.3. He at surfaces

Experimental results show that He forms bubbles at the near surface in the range 0–2  $\mu\text{m}$  [34,35]. Therefore, the surface effect is very important for understanding the He behaviors in W. We have investigated the dissolution and clustering of He at W (1 1 0) surface [36]. It is found that a single He is not energetically favorable sitting at both the surface and the subsurface, but it can stably stay under the second atomic layer form the surface. This is also can be attributed to the special electronic structure of He, leading to the interaction between He and W is very weak. The solution energy of He is  $\sim 6.1$  eV at the surface, which is almost similar with that of He in the bulk. Further, it is found that two He atoms can attract with each other within certain distance at different layers with a binding energy of  $\sim 1.0$  eV. This suggests that He atom prefers to form He clusters at the near surface. In addition, the clustering of multiple He atoms will produce at the surface and form He-vacancy complex.

## 4. Effects of impurity and alloying element on He behaviors

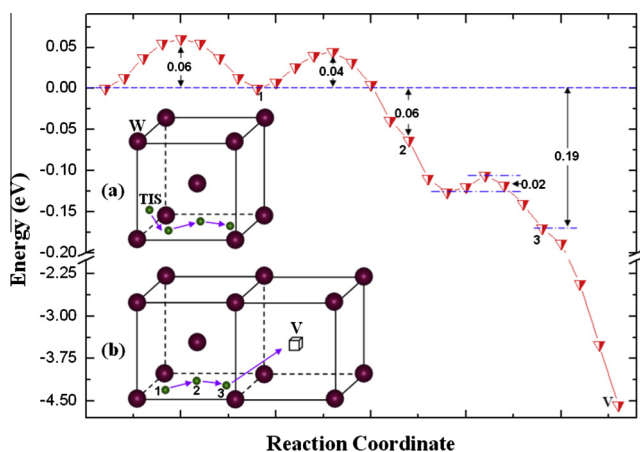
### 4.1. Effects of carbon on He behaviors

Carbon (C) is commonly considered as one of the most frequent impurity in W. It is expected to plays a key role in the energetics and kinetics of defects, though C is present only very small amount [3,37,38]. Therefore, C could be expected to have a crucial influence on the He retention and diffusion in W. We have investigated the effect of C on He in W [39]. A single C prefers to occupy the OIS in the bulk W, while a He atom is favorable sitting at TIS. In order to investigate the effect of interstitial C atom on the He in the bulk W, one C atom is set at an OIS while the He atom occupies a different TIS. It is found that there is an attraction between C and He with a binding energy of  $\sim 0.41$  eV. Therefore, the pre-existing C atom can largely reduce the solution energy of He, which indicates that interstitial C can serve as a trapping centre of He in W. This can be attributed to the volume expansion of the local OIS with C, which leads to further expansion of the neighboring TIS's. Therefore, the lower electron density in TIS surrounding C due to the volume expansion can reduce the solution energy of He.

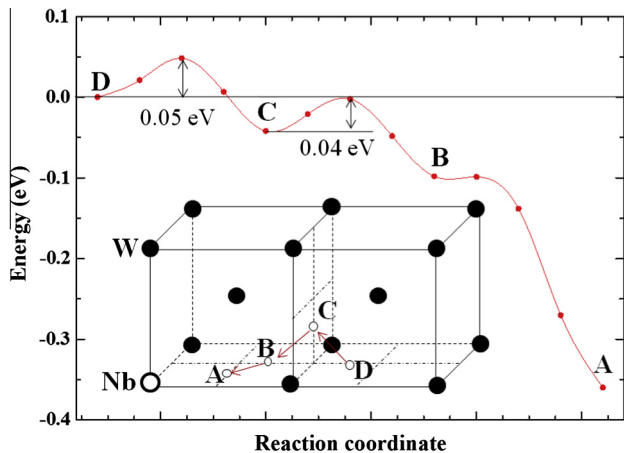
Previous studies have demonstrated that a vacancy can serve as trapping center for C and He in W. Thus, with the pre-existing C impurity in W, a C–vacancy (C–V) complex maybe can also serve as a trapping center for He. The solution energy of a single He at C–V complex is much lower than that of He in bulk W, which suggests imply that the C–V complex can act as a trapping center and drives segregation of He towards it. Further, although the solution energy at C–V complex is much low than that at TIS in bulk, it is higher than that at C–free vacancy, which indicate the He trapping capability of C–V complex is weaker than that of the C–free vacancy. For the case of multiple He atoms, it is found that one C–V complex can trap five He atoms, less than the maximum number of He atoms trapped by one C–free vacancy. These also indicate that the pre-existing C atom will reduce the He trapping capability of vacancy.

### 4.2. Effects of niobium on He behaviors

The addition of alloying element niobium (Nb) is one well-known method to enhance the mechanical properties of W. The existing of Nb will have effect on He in W. Therefore, we have



**Fig. 5.** He diffusion energy profile and diffusion paths (arrows) in W. (a) He diffusion from one TIS to another in the intrinsic bulk W, via the TIS  $\rightarrow$  TIS path. (b) He diffusion towards an empty vacancy, via the path from the 3NN (site 1), 2NN TIS (site 2) to 1NN (site 3) TIS of the vacancy. Site 1, 2 and 3 are the 3NN, 2NN and 1NN TIS of the vacancy, respectively [31].



**Fig. 6.** He diffusion towards a Nb atom, via the path from the 4NN (site D), 3NN TIS (site C), 2NN TIS (site B) to 1NN (site A) TIS of the Nb. Site D, C, B and A are the 4NN, 3NN, 2NN and 1NN TIS of the Nb, respectively [40].

investigated the interaction between He and Nb in W [40]. It is found that Nb can effectively reduce the solution energy of He in bulk W, which can be attributed to the electron density redistribution. The most stable site of He in W–Nb is the 1NN TIS from Nb, corresponding to solution energy of 5.74 eV. The solution energy increases with increasing Nb–He distance, and converges to that of He at TIS in bulk W. Thus, Nb can serve as a He trapping centre in W with the trapping energy of 0.37 eV. Further, as shown in Fig. 6, it is found that the diffusion barrier of He towards Nb will decrease with the decreasing of Nb–He distance, which suggests that He can very easily diffuse to Nb in W. Therefore, it can be expected that the presence of Nb will facilitate the nucleation and blistering of He in W.

## 5. Summary

In summary, we have investigated the behavior of He in W using a first-principles method, which can contribute to the design and application of W materials as a PFM under a fusion environment. So far, our main data have been obtained using first-principles calculations, which have limitations and in particular the effect of temperature. For the future, we will further investigate the physical mechanism of the accumulation of He and the growth of He bubbles in W employing various computational methods with different space and time scale. This will provide useful reference to further understand the different behavior of He in W, triggering at the design of plasma-irradiation-resistant materials.

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